

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102620\
 Data File : VU040950.D
 Acq On : 26 Oct 2020 17:34
 Operator : SY/MD
 Sample : L4492-05
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN3

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.362	3	7	23	rVB	97385	94528	27.47%	3.664%
2	1.478	36	43	46	rBV	35124	36649	10.65%	1.420%
3	1.604	71	82	94	rBV3	52474	80031	23.26%	3.102%
4	1.739	116	124	135	rVB	25932	31590	9.18%	1.224%
5	1.922	173	181	193	rVB	23148	31211	9.07%	1.210%
6	2.002	198	206	219	rBV	13193	18280	5.31%	0.708%
7	2.166	249	257	264	rVV	8618	11657	3.39%	0.452%
8	2.215	264	272	281	rVB2	7865	11241	3.27%	0.436%
9	2.420	331	336	346	rVB5	2339	3506	1.02%	0.136%
10	2.578	373	385	399	rBV	39491	63728	18.52%	2.470%
11	2.687	402	419	427	rBV	4688	13869	4.03%	0.538%
12	3.202	565	579	595	rVB2	16551	37760	10.97%	1.463%
13	4.674	1018	1037	1109	rBV2	44656	255864	74.36%	9.916%
14	5.083	1146	1164	1185	rVB	42820	95252	27.68%	3.692%
15	5.742	1348	1369	1379	rBV2	78474	209739	60.96%	8.129%
16	6.263	1518	1531	1544	rBV	75736	139876	40.65%	5.421%
17	6.703	1655	1668	1682	rBV	53054	101090	29.38%	3.918%
18	6.774	1682	1690	1701	rVB7	3582	7011	2.04%	0.272%
19	7.574	1926	1939	1953	rBV	23897	40715	11.83%	1.578%
20	7.906	2030	2042	2054	rBV	80414	134467	39.08%	5.211%
21	7.976	2054	2064	2077	rVB	40579	69932	20.32%	2.710%
22	8.185	2119	2129	2143	rBV	16444	26485	7.70%	1.026%
23	8.642	2257	2271	2305	rBV	179675	344077	100.00%	13.335%
24	8.790	2307	2317	2330	rVB3	13157	22005	6.40%	0.853%
25	9.420	2501	2513	2532	rBV	113430	182348	53.00%	7.067%
26	9.568	2552	2559	2567	rBV2	2245	3449	1.00%	0.134%
27	9.690	2587	2597	2607	rVB2	7959	11642	3.38%	0.451%
28	10.102	2711	2725	2732	rBV2	5578	8340	2.42%	0.323%
29	10.233	2758	2766	2778	rBB3	2918	4465	1.30%	0.173%
30	10.754	2917	2928	2941	rBV	47369	75753	22.02%	2.936%
31	11.809	3245	3256	3269	rBV	100956	158642	46.11%	6.148%
32	12.053	3321	3332	3352	rBV	39222	76626	22.27%	2.970%
33	12.188	3362	3374	3386	rVB	97063	151987	44.17%	5.890%
34	12.764	3546	3553	3559	rBV5	3070	4039	1.17%	0.157%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Title : TRACE VOA SOM01.0

35	12.880	3579	3589	3601	rVB4	4120	5870	1.71%	0.227%
36	15.208	4305	4313	4323	rBV2	6107	9298	2.70%	0.360%
37	15.394	4361	4371	4383	rVB	4898	7240	2.10%	0.281%

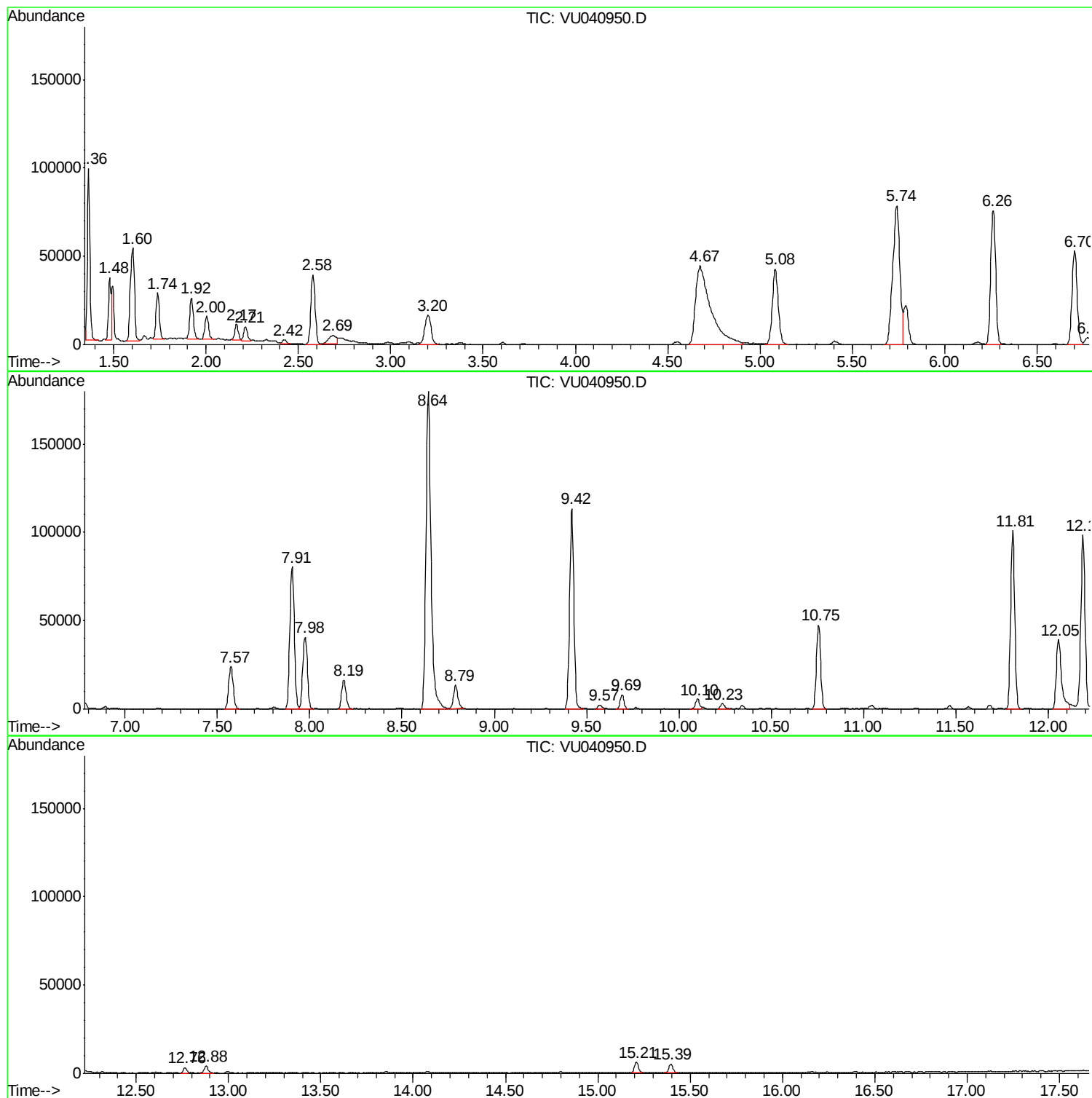
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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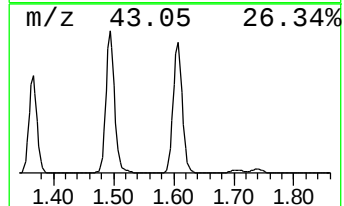
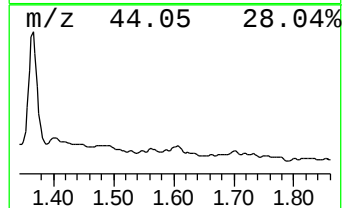
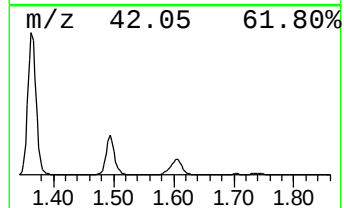
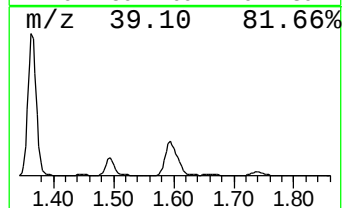
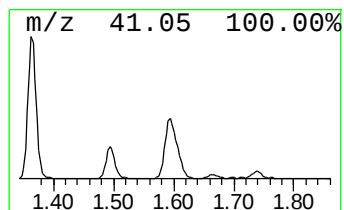
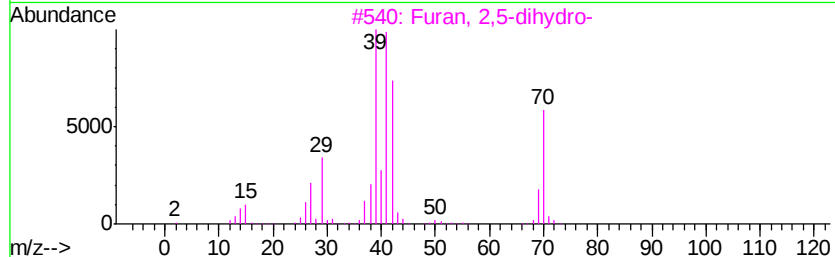
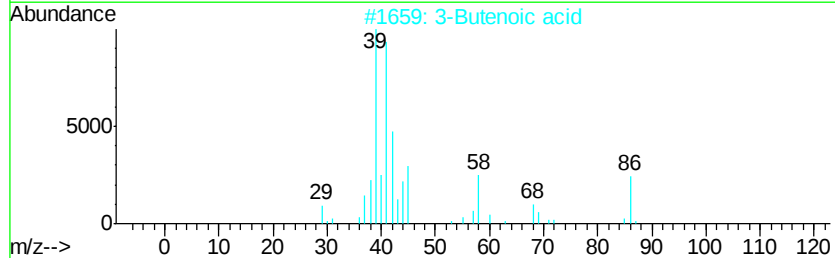
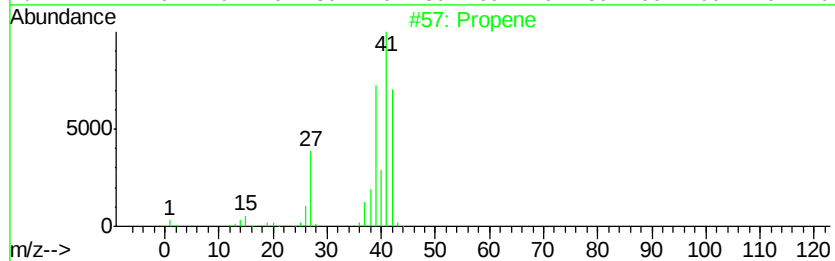
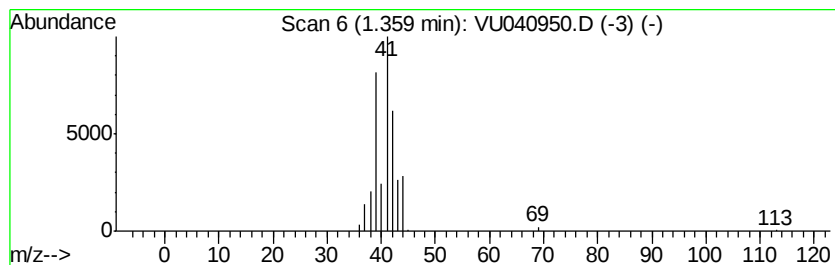
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
1.36	3.38 ug/L	94528	1,4-Difluorobenzene	6.26		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene		42	C3H6	000115-07-1	90
2	3-Butenoic acid		86	C4H6O2	000625-38-7	83
3	Furan, 2,5-dihydro-		70	C4H6O	001708-29-8	83
4	2-Butenal, (E)-		70	C4H6O	000123-73-9	78
5	Cycloheptano[d]imidazolidine, 1,...		186	C9H18N2O2	306947-39-7	74



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Instrument :
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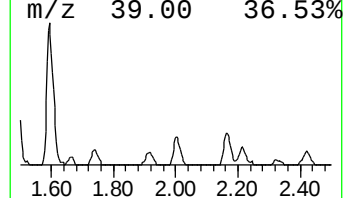
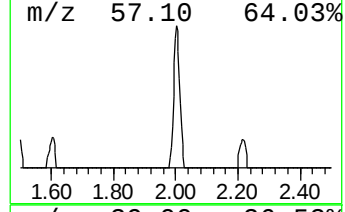
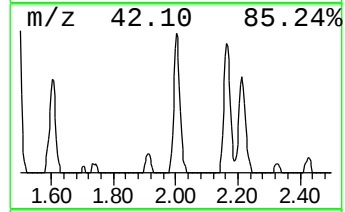
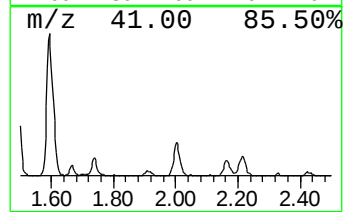
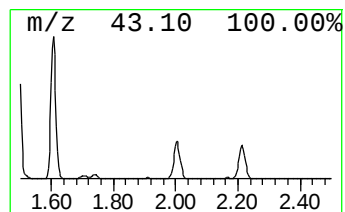
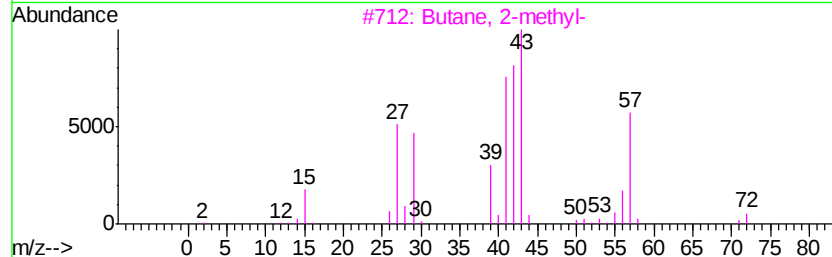
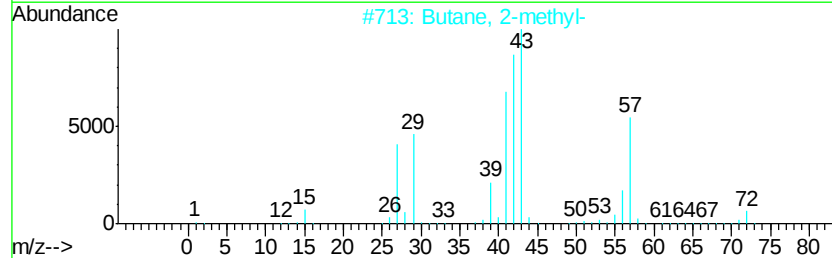
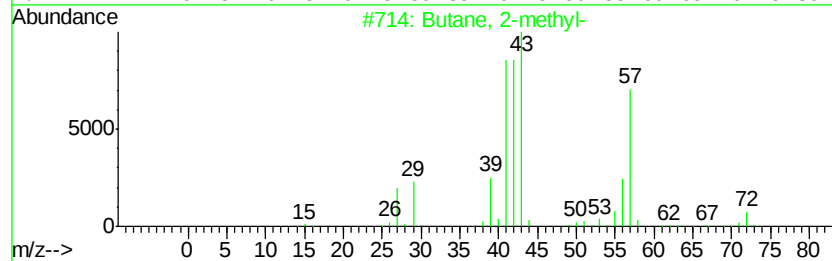
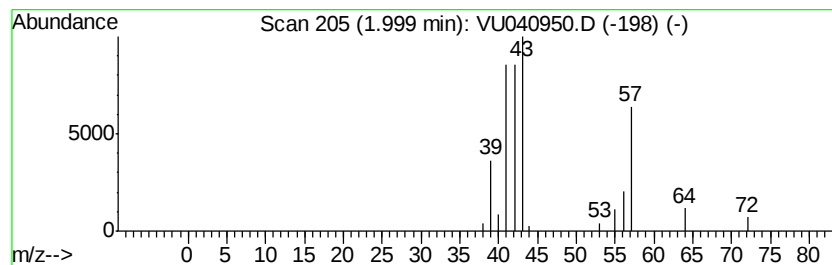
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	0.65 ug/L	18280	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2		Butane, 2-methyl-	72	C5H12	000078-78-4	90
3		Butane, 2-methyl-	72	C5H12	000078-78-4	86
4		Pentane	72	C5H12	000109-66-0	39
5		3-Buten-1-ol	72	C4H8O	000627-27-0	9



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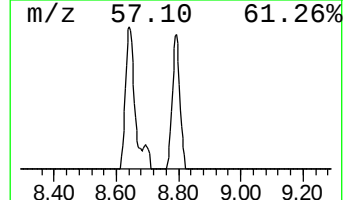
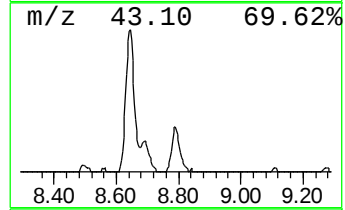
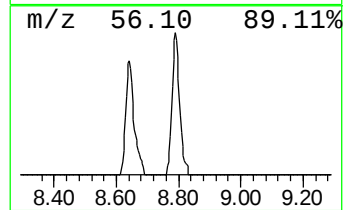
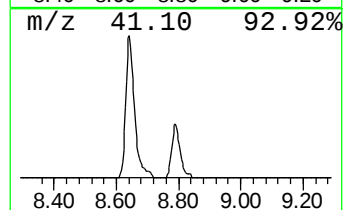
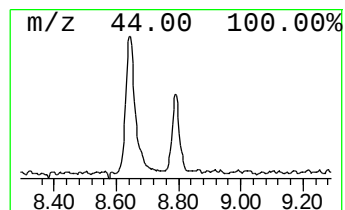
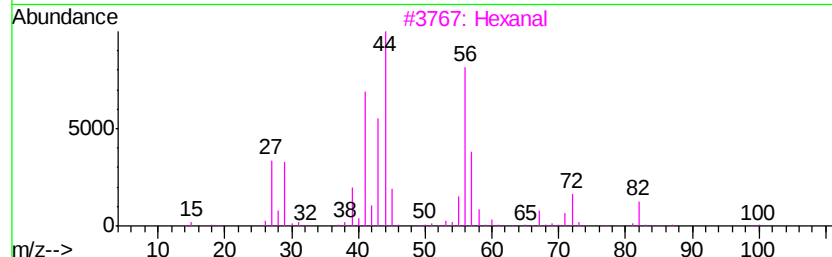
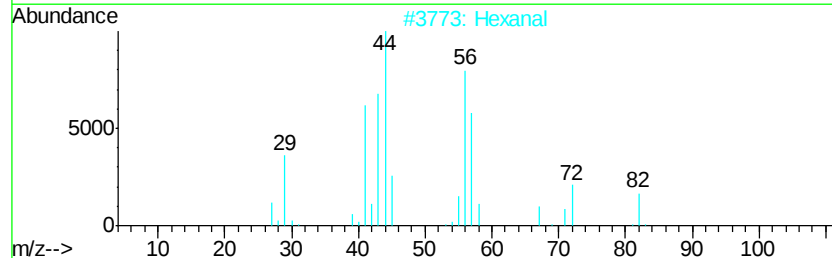
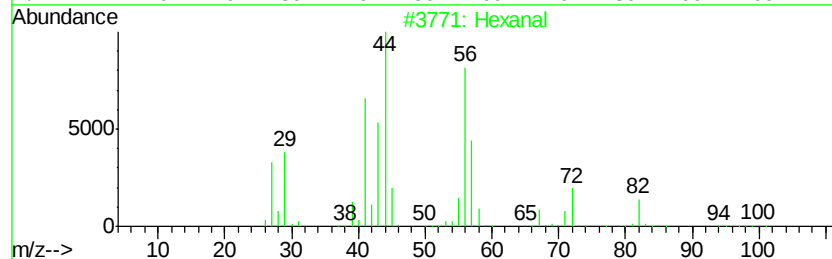
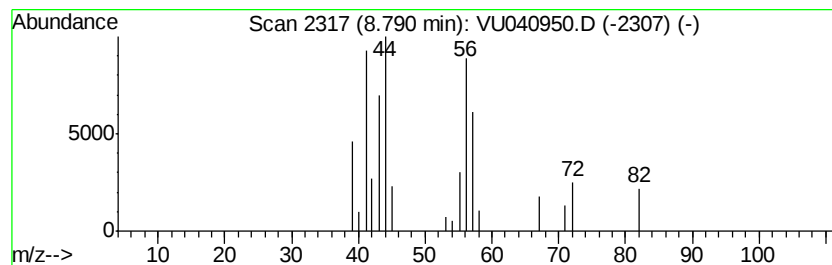
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.79	0.60 ug/L	22005	Chlorobenzene-d5	9.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	64
2		Hexanal	100	C6H12O	000066-25-1	64
3		Hexanal	100	C6H12O	000066-25-1	59
4		Hexanal	100	C6H12O	000066-25-1	53
5		Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	33



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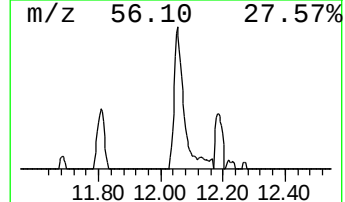
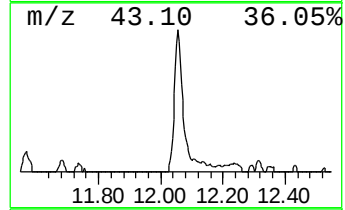
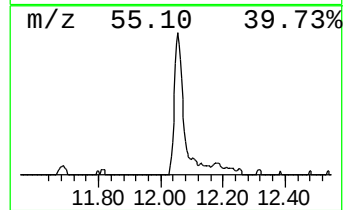
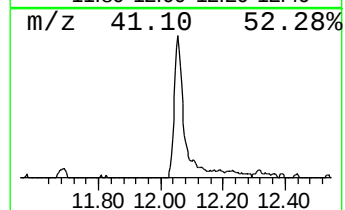
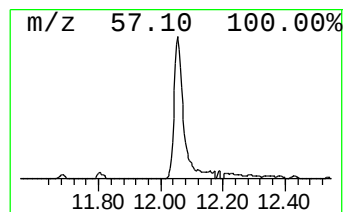
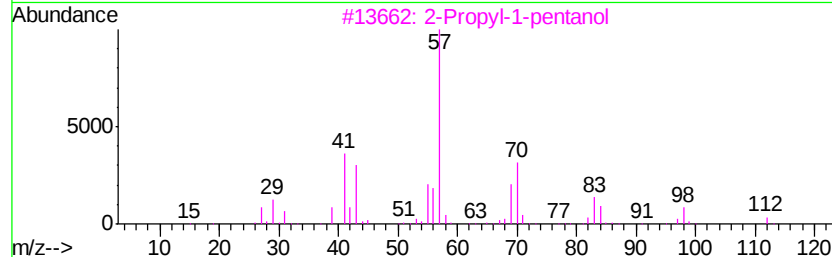
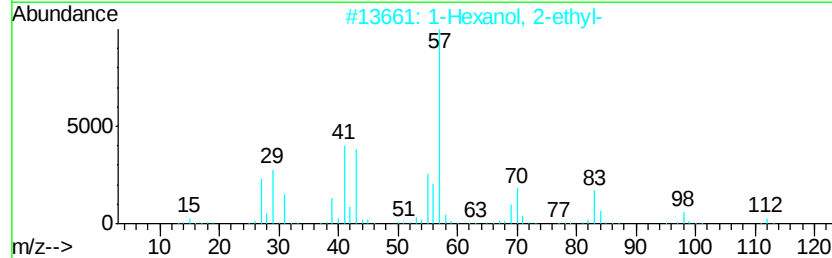
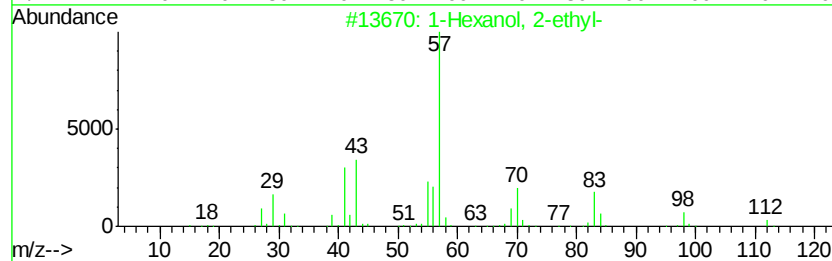
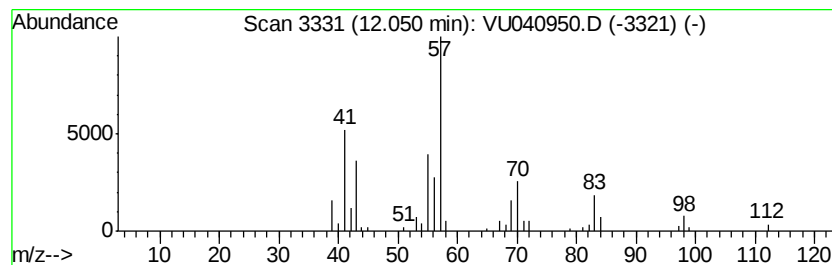
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	2.42 ug/L	76626	1,4-Dichlorobenzene-d4	11.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Str...	1.36	3.4	ug/L	94528	1	6.26	139876	5.0
(DEL) Alkane: Str...	2.00	0.7	ug/L	18280	1	6.26	139876	5.0
Hexanal	8.79	0.6	ug/L	22005	2	9.42	182348	5.0
1-Hexanol, 2-ethyl-	12.05	2.4	ug/L	76626	3	11.81	158642	5.0